

# SEPARABILITY OF THREE QUBIT GREENBERGER-HORNE-ZEILINGER DIAGONAL STATES

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**ABSTRACT.** We characterize the separability of three qubit GHZ diagonal states in terms of entries. This enables us to check separability of GHZ diagonal states without decomposition into the sum of pure product states. In the course of discussion, we show that the necessary criterion of Gühne [1] for (full) separability of three qubit GHZ diagonal states is sufficient with a simpler formula. The main tool is to use entanglement witnesses which are tri-partite Choi matrices of positive bi-linear maps.

## 1. INTRODUCTION

Entanglement is now considered as one of the most important resources in quantum information theory, and it is crucial to detect entanglement from separability. Positivity of partial transposes is a simple but powerful criterion for separability [2, 3]. In fact, it is known [4, 5] that PPT property is equivalent to separability for  $2 \otimes 2$  or  $2 \otimes 3$  systems. But, it is very difficult in general to distinguish separability from entanglement, as it is known to be an *NP*-hard problem [6].

The purpose of this note is to give a complete characterization of separability for three qubit Greenberger-Horne-Zeilinger diagonal states, which are diagonal in the GHZ basis. Those include mixtures of GHZ states and identity, as they were considered in [7, 8] for examples. In multi-qubit systems, GHZ states [9, 10] are key examples of maximally entangled states, and they are known to have many applications in quantum information theory. They also play central roles in the classification of multi-qubit entanglement [7, 11, 12]. See survey articles [13, 14] for general theory of entanglement as well as various aspects of GHZ states.

Our main tool is to use the notion of entanglement witnesses. In the bi-partite cases, positive linear maps are very useful to detect entanglement through the duality between tensor products and linear maps [5, 15]. This duality has been formulated as the notion of entanglement witnesses [16], which is still valid in multi-partite cases. In the tri-partite cases, the second author [17] has interpreted entanglement witnesses as positive bi-linear maps. With this interpretation, we carefully choose useful entanglement witnesses for our purpose.

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There were two major steps to characterize separability of three qubit GHZ diagonal states in the literature. Kay [18] gave a condition under which a GHZ diagonal state is separable if and only if it is of positive partial transpose. On the other hand, Gühne [1] gave a necessary criterion for separability of three qubit GHZ diagonal states, and provided a sufficient condition for separability. We will describe their results after we give definitions and fix notations in the next section, where we will also explain what is our work precisely.

## 2. GHZ DIAGONAL STATES

We recall that a state is (fully) separable if it is a convex combination of pure product states, and entangled if it is not separable. So, a three qubit state  $\varrho$  in the tensor product  $M_2 \otimes M_2 \otimes M_2$  is separable if and only if it can be written by the finite sum of the form

$$\varrho = \sum_i p_i |\xi_i\rangle \otimes |\eta_i\rangle \otimes |\zeta_i\rangle \langle \xi_i| \otimes \langle \eta_i| \otimes \langle \zeta_i|$$

with  $p_i > 0$ ,  $\sum_i p_i = 1$  and two dimensional vectors  $|\xi_i\rangle$ ,  $|\eta_i\rangle$  and  $|\zeta_i\rangle$ . Throughout this paper, three qubit states will be considered as  $8 \times 8$  matrices with the identification  $M_2 \otimes M_2 \otimes M_2 = M_8$  through the lexicographic order of indices in the tensor product. We may take some subsystems and take the transposes for them to get partial transposes. For example, we take the first system, then the corresponding partial transpose of a three qubit product state  $x \otimes y \otimes z$  is given by  $x^t \otimes y \otimes z$ . The PPT criteria [2, 3] tell us that if  $\varrho$  is separable then all the partial transposes of  $\varrho$  are positive.

The three qubit GHZ state basis consists of eight vectors in  $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$  given by

$$|\xi_{ijk}\rangle = \frac{1}{\sqrt{2}} (|i\rangle \otimes |j\rangle \otimes |k\rangle + (-1)^i |\bar{i}\rangle \otimes |\bar{j}\rangle \otimes |\bar{k}\rangle), \quad i + \bar{i} = 1 \pmod{2},$$

where the index  $ijk$  runs through  $i, j, k \in \{0, 1\}$ . We endow the indices with the lexicographic order to get eight vectors  $\xi_1, \xi_2, \dots, \xi_8$ . A GHZ diagonal state is of the form

$$\varrho = \sum_{i=1}^8 p_i |\xi_i\rangle \langle \xi_i|$$

for nonnegative  $p_i$ 's with  $\sum_{i=1}^8 p_i = 1$ . Then we see that  $2\varrho$  is written as the following  $8 \times 8$  matrix:

$$X(a, b, c) := \begin{pmatrix} a_1 & & & & & & & c_1 \\ & a_2 & & & & & & c_2 \\ & & a_3 & & & & & c_3 \\ & & & a_4 & c_4 & & & \\ & & & \bar{c}_4 & b_4 & & & \\ & & & & & b_3 & & \\ & & \bar{c}_3 & & & & b_2 & \\ & \bar{c}_2 & & & & & & b_1 \\ \bar{c}_1 & & & & & & & \end{pmatrix},$$

whose entries are all zero except for diagonal and anti-diagonal entries with

$$\begin{aligned} a = b &= (p_1 + p_8, p_2 + p_7, p_3 + p_6, p_4 + p_5) \in \mathbb{R}^4, \\ c &= (p_1 - p_8, p_2 - p_7, p_3 - p_6, p_4 - p_5) \in \mathbb{R}^4. \end{aligned}$$

The self-adjoint matrix of the form  $X(a, b, c)$  with  $a, b \in \mathbb{R}^4$  and  $c \in \mathbb{C}^4$  is called X-shaped. Therefore, we have seen that a three qubit GHZ diagonal state is an X-shaped state, or X-state in short,  $X(a, b, c)$  with  $a, b \in \mathbb{R}^4$  and  $c \in \mathbb{R}^4$ . Conversely, every X-state  $X(a, b, c)$  can be realized as a GHZ diagonal state whenever  $a = b$  and  $c \in \mathbb{R}^4$ . A mixture of  $|\xi_1\rangle\langle\xi_1|$  and the identity is the simplest example of a nontrivial GHZ diagonal state, as it was considered in [8]. Dür, Cirac and Tarrach [7] considered GHZ diagonal states with  $c = (c_1, 0, 0, 0)$ , and showed that these states are separable if and only if they are of PPT. See also [12] for multi-qubit analogues. On the other hand, X-states with  $a_i b_i = 1$  and  $c = (1, 0, 0, 0)$  were considered [11] in the contexts of classification of three qubit PPT entangled edge states. See also [19] for criteria for separability of three qubit states by their X-parts.

There are other expression [20] of GHZ diagonal states, using Pauli matrices

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

If  $a = b$  and  $c \in \mathbb{R}^4$ , then a GHZ diagonal state  $\varrho = X(a, a, c)$  can be written as

$$\begin{aligned} X(a, a, c) &= \frac{1}{8} (I \otimes I \otimes I + \lambda_2 Z \otimes Z \otimes I + \lambda_3 Z \otimes I \otimes Z + \lambda_4 I \otimes Z \otimes Z \\ &\quad + \lambda_5 X \otimes X \otimes X + \lambda_6 Y \otimes Y \otimes X + \lambda_7 Y \otimes X \otimes Y + \lambda_8 X \otimes Y \otimes Y), \end{aligned}$$

with the coefficients

$$\begin{aligned} \lambda_2 &= 2(+a_1 + a_2 - a_3 - a_4), \\ \lambda_3 &= 2(+a_1 - a_2 + a_3 - a_4), & \lambda_4 &= 2(+a_1 - a_2 - a_3 + a_4), \\ \lambda_5 &= 2(+c_1 + c_2 + c_3 + c_4), & \lambda_6 &= 2(-c_1 - c_2 + c_3 + c_4), \\ \lambda_7 &= 2(-c_1 + c_2 - c_3 + c_4), & \lambda_8 &= 2(-c_1 + c_2 + c_3 - c_4). \end{aligned} \tag{1}$$

Now, we are ready to describe the results on the separability of a three qubit state  $\varrho = X(a, a, c)$  by Kay [18] and Gühne [1]:

- If  $\prod_{i=5}^8 \lambda_i \leq 0$ , then  $\varrho$  is separable if and only if  $\varrho$  is of PPT [18].
- If  $\prod_{i=5}^8 \lambda_i > 0$ , then the inequality

$$\min\{a_1, a_2, a_3, a_4\} \geq \frac{\sqrt{(\lambda_5 \lambda_6 + \lambda_7 \lambda_8)(\lambda_5 \lambda_7 + \lambda_6 \lambda_8)(\lambda_5 \lambda_8 + \lambda_6 \lambda_7)}}{8\sqrt{\lambda_5 \lambda_6 \lambda_7 \lambda_8}} \tag{2}$$

implies the separability of  $\varrho$  [1].

Kay [18] also considered the state  $\varrho = X(a, a, c)$  with  $a = (4 + \alpha, \alpha, \alpha, \alpha)$  and  $c = (2, 2, -2, 2)$  to give examples of PPT entangled states among GHZ diagonal states. Our main contribution is to give a condition in terms of anti-diagonal entries of  $\varrho$  with the following properties:

- If  $\varrho$  satisfies this condition, then  $\varrho$  is separable if and only if  $\varrho$  satisfies (2).

- If  $\varrho$  does not meet this condition, then  $\varrho$  is separable if and only if  $\varrho$  is of PPT.

See Theorem 5.2 for the precise description of this condition. This completes the characterization of separability of three qubit GHZ diagonal states in terms of entries. This is one of few cases in the literature where the separability problem is solved in terms of entries. With this characterization, we may confirm the separability of a GHZ diagonal state without a concrete decomposition into the sum of pure product states, which is usually a quite nontrivial job.

Suppose that the X-part of a three qubit state  $\varrho$  is given by  $X(a, b, c)$  with  $a, b \in \mathbb{R}^4$  and  $c \in \mathbb{C}^4$ . In order to get a necessary condition for separability of GHZ diagonal states, Gühne [1] also introduced the following:

$$\begin{aligned}\mathcal{L}(\varrho, z) &:= \text{Re}(z_1 c_1 + z_2 c_2 + z_3 c_3 + z_4 \bar{c}_4), \quad z \in \mathbb{C}^4 \\ \mathcal{F}(z) &:= \text{Re}(z_1) \cos(\alpha + \beta + \gamma) - \text{Im}(z_1) \sin(\alpha + \beta + \gamma) + \text{Re}(z_2) \cos(\alpha) - \text{Im}(z_2) \sin(\alpha) \\ &\quad + \text{Re}(z_3) \cos(\beta) - \text{Im}(z_3) \sin(\beta) + \text{Re}(z_4) \cos(\gamma) - \text{Im}(z_4) \sin(\gamma), \\ C(z) &:= \sup_{\alpha, \beta, \gamma} |\mathcal{F}(z)|\end{aligned}$$

and showed that if  $\varrho = X(a, b, c)$  is separable then the inequality

$$(3) \quad \mathcal{L}(\varrho, z) \leq C(z) \Delta_\varrho$$

holds for every  $z \in \mathbb{C}^4$ , where the number  $\Delta_\varrho$  is given by

$$\Delta_\varrho = \min \left\{ \sqrt{a_i b_i} \ (i = 1, 2, 3, 4), \ \sqrt[4]{a_1 b_2 b_3 a_4}, \ \sqrt[4]{b_1 a_2 a_3 b_4} \right\}$$

which is determined by the diagonal entries of  $\varrho = X(a, b, c)$ . If  $\varrho$  is GHZ diagonal, then we have  $\Delta_\varrho = \min\{a_1, a_2, a_3, a_4\}$ . The number  $C(z)$  above turns out to coincide essentially with the number in the characterization of three qubit X-shaped entanglement witnesses [21]. In this way, we got a simpler expression for  $C(z)$ . See Proposition 3.4.

In the next section, we will also consider X-shaped entanglement witnesses, and show that special kinds of them are enough to confirm the separability of GHZ diagonal states. These will be used in Section 4 to prove our result that Gühne's necessary condition is also sufficient for separability of three qubit GHZ diagonal states. In Section 5, we apply this condition to give a concrete entry-wise characterization of separability for three qubit GHZ diagonal states.

### 3. ENTANGLEMENT WITNESSES

We recall that a non-positive self-adjoint matrix  $W$  in  $M_A \otimes M_B \otimes M_C$  is an entanglement witness if

$$\langle \varrho, W \rangle := \text{Tr}(\varrho W^t) \geq 0$$

for every separable state  $\varrho$ . A matrix  $W$  in  $M_A \otimes M_B \otimes M_C$  is written by

$$\begin{aligned} W &= \sum_{i_1, j_1} |i_1\rangle\langle j_1| \otimes W_{i_1, j_1} \in M_A \otimes (M_B \otimes M_C) \\ &= \sum_{i_1, j_1} \sum_{i_2, j_2} |i_1\rangle\langle j_1| \otimes |i_2\rangle\langle j_2| \otimes W_{i_1 i_2, j_1 j_2} \in M_A \otimes M_B \otimes M_C \end{aligned}$$

in a unique way, and so we may associate a bi-linear map  $\phi_W : M_A \times M_B \rightarrow M_C$  by

$$\phi_W(|i_1\rangle\langle j_1|, |i_2\rangle\langle j_2|) = W_{i_1 i_2, j_1 j_2}$$

for matrix units  $\{|i_1\rangle\langle j_1|\}$  and  $\{|i_2\rangle\langle j_2|\}$  of  $M_A$  and  $M_B$ , respectively. It is known [17] that  $\langle \varrho, W \rangle \geq 0$  for every separable state  $\varrho$  if and only if  $\phi_W$  is a positive bi-linear map, that is,  $\phi(x, y) \in M_C$  is positive whenever  $x \in M_A$  and  $y \in M_B$  are positive.

For a given  $|x\rangle = (x_0, x_1)^t \in \mathbb{C}^2$ , we write  $|x_\pm\rangle = (x_0, \pm x_1)^t$ . Then the X-part of the pure product state  $\varrho = |\xi\rangle\langle\xi|$  with  $|\xi\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle$  is given by the average of the four pure product states:  $\varrho_X = \frac{1}{4} \sum_{k=0}^3 |\xi_k\rangle\langle\xi_k|$ , where  $|\xi_k\rangle$  is given by

$$\begin{aligned} |\xi_0\rangle &= |x_+\rangle \otimes |y_+\rangle \otimes |z_+\rangle, \\ |\xi_1\rangle &= |x_+\rangle \otimes |y_-\rangle \otimes |z_-\rangle, \\ |\xi_2\rangle &= |x_-\rangle \otimes |y_+\rangle \otimes |z_-\rangle, \\ |\xi_3\rangle &= |x_-\rangle \otimes |y_-\rangle \otimes |z_+\rangle. \end{aligned}$$

Therefore, we see that the X-part of a separable state is again separable. This simple observation has an important implication.

**Proposition 3.1.** *The X-part of a three qubit entanglement witness is still an entanglement witness unless it is positive.*

*Proof.* We denote by  $W_X$  and  $\varrho_X$  the X-parts of an entanglement witness  $W$  and a state  $\varrho$ , respectively. Suppose that  $\varrho$  is separable. Then we have  $\langle \varrho, W_X \rangle = \langle \varrho_X, W \rangle \geq 0$ , because  $\varrho_X$  is separable. This shows that  $W_X$  is an entanglement witness.  $\square$

We say that an X-shaped self-adjoint matrix  $W = X(s, t, u)$  is *GHZ diagonal* if  $s = t$  and  $u \in \mathbb{R}$ .

**Theorem 3.2.** *Let  $\varrho$  be a GHZ diagonal state. Then,  $\varrho$  is separable if and only if  $\langle \varrho, W \rangle \geq 0$  for every GHZ diagonal witness  $W$ .*

*Proof.* The ‘only if’ part is clear. For the ‘if’ part, it suffices to show that  $\langle \varrho, W \rangle \geq 0$  for every X-shaped witness  $W$  by Proposition 3.1. We consider the operation on  $M_2 \otimes M_2 \otimes M_2$  which interchanges  $|0\rangle$  and  $|1\rangle$  in each subsystem. This operation sends an entanglement witness  $W = X(s, t, u)$  to the entanglement witness  $\widetilde{W} = X(t, s, \bar{u})$ . Explicitly, we can write  $\widetilde{W} = UWU^*$  for the symmetric unitary

$$U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The average

$$\frac{W + \widetilde{W}}{2} = X\left(\frac{s+t}{2}, \frac{s+t}{2}, \text{Re } u\right)$$

is GHZ diagonal, and  $W$  is GHZ diagonal if and only if  $(W + \widetilde{W})/2 = W$ . In other words, the mapping  $W \mapsto (W + \widetilde{W})/2$  is an idempotent from the real space of X-shaped self-adjoint matrices onto its subspace consisting of GHZ diagonal matrices. We have

$$\begin{aligned} \langle \varrho, W \rangle &= \left\langle \frac{\varrho + \widetilde{\varrho}}{2}, W \right\rangle \\ &= \frac{1}{2} (\langle \varrho, W \rangle + \text{Tr}(U \varrho U^* W^t)) \\ &= \frac{1}{2} (\langle \varrho, W \rangle + \text{Tr}(\varrho(UWU^*)^t)) = \left\langle \varrho, \frac{W + \widetilde{W}}{2} \right\rangle \geq 0, \end{aligned}$$

which completes the proof.  $\square$

For a three qubit X-shaped self-adjoint matrix  $W = X(s, t, u)$ , the authors [21] have shown that  $W = X(s, t, u)$  is an entanglement witness if and only if it is non-positive and satisfies the inequality

$$\begin{aligned} &\sqrt{(s_1 + t_4|\alpha|^2)(s_4 + t_1|\alpha|^2)} + \sqrt{(s_2 + t_3|\alpha|^2)(s_3 + t_2|\alpha|^2)} \\ &\geq |u_1\bar{\alpha} + \bar{u}_4\alpha| + |u_2\bar{\alpha} + \bar{u}_3\alpha| \end{aligned}$$

for each complex number  $\alpha \in \mathbb{C}$ . If we write  $\alpha = re^{i\theta}$ , then the above inequality is equivalent to the following

$$\begin{aligned} &\sqrt{(s_1r^{-1} + t_4r)(s_4r^{-1} + t_1r)} + \sqrt{(s_2r^{-1} + t_3r)(s_3r^{-1} + t_2r)} \\ &\geq |u_1e^{-i\theta} + \bar{u}_4e^{i\theta}| + |u_2e^{-i\theta} + \bar{u}_3e^{i\theta}|, \end{aligned}$$

which holds for every  $r > 0$  and  $\theta$ . For a given  $(s, t) \in \mathbb{R}_+^4 \times \mathbb{R}_+^4$  and  $u \in \mathbb{C}^4$ , we introduce two numbers:

$$\begin{aligned} A(s, t) &= \inf_{r>0} \left[ \sqrt{(s_1r^{-1} + t_4r)(s_4r^{-1} + t_1r)} + \sqrt{(s_2r^{-1} + t_3r)(s_3r^{-1} + t_2r)} \right], \\ B(u) &= \max_{\theta} (|u_1e^{i\theta} + \bar{u}_4| + |u_2e^{i\theta} + \bar{u}_3|). \end{aligned}$$

Here,  $\mathbb{R}_+$  denotes the interval  $[0, \infty)$ . Then we have the following:

**Proposition 3.3.** *A three qubit non-positive self-adjoint matrix  $W = X(s, t, u)$  is an entanglement witness if and only if the inequality  $A(s, t) \geq B(u)$  holds.*

It is surprising to note that the number  $B(u)$  is essentially identical with the number  $C(z)$  in the Gühne's criterion. This enables us to calculate the number  $C(z)$  in terms of entries of  $z$ .

**Proposition 3.4.** *For  $z \in \mathbb{C}^4$ , we have  $C(z) = B(z_1, z_2, z_3, \bar{z}_4)$ .*

*Proof.* We have

$$\begin{aligned}
\mathcal{F}(z) &= \operatorname{Re} (z_1 e^{i(\alpha+\beta+\gamma)} + z_2 e^{i\alpha} + z_3 e^{i\beta} + z_4 e^{i\gamma}) \\
&= \operatorname{Re} (z_1 e^{i(\alpha+\beta+\gamma)} + z_2 e^{i\alpha} + \bar{z}_3 e^{-i\beta} + z_4 e^{i\gamma}) \\
&\leq |z_1 e^{i(\alpha+\beta+\gamma)} + z_4 e^{i\gamma}| + |z_2 e^{i\alpha} + \bar{z}_3 e^{-i\beta}| \\
&= |z_1 e^{i(\alpha+\beta)} + z_4| + |z_2 e^{i(\alpha+\beta)} + \bar{z}_3| \\
&\leq \max_{\theta} |z_1 e^{i\theta} + z_4| + |z_2 e^{i\theta} + \bar{z}_3|.
\end{aligned}$$

For the converse, we put  $\phi := -\arg(z_1 e^{i\theta} + z_4)$  and  $\psi := -\arg(z_2 e^{i\theta} + \bar{z}_3)$ . Then, we have

$$\begin{aligned}
|z_1 e^{i\theta} + z_4| + |z_2 e^{i\theta} + \bar{z}_3| &= \operatorname{Re} ((z_1 e^{i\theta} + z_4) e^{i\phi}) + \operatorname{Re} ((z_2 e^{i\theta} + \bar{z}_3) e^{i\psi}) \\
&= \operatorname{Re} (z_1 e^{i(\theta+\phi)} + z_2 e^{i(\theta+\psi)} + z_3 e^{-i\psi} + z_4 e^{i\phi}) \\
&\leq C(z),
\end{aligned}$$

where the last inequality follows from  $(\theta + \psi) - \psi + \phi = \theta + \phi$ .  $\square$

#### 4. A PROOF OF GÜHNE'S CONJECTURE

In this section, we show that Gühne's necessary condition (3) is also sufficient for separability of GHZ diagonal states. We begin with a characterization of separability of general X-shaped states.

**Proposition 4.1.** *Let  $\varrho$  be a three qubit state whose X-part is given by  $X(a, b, c)$ . If  $\varrho$  is separable, then the inequality*

$$2A(x, y)\mathcal{L}(\varrho, z) \leq C(z) \left( \sum_{i=1}^4 a_i x_i + \sum_{i=1}^4 b_i y_i \right)$$

holds for every  $x, y \in \mathbb{R}_+^4$  and  $z \in \mathbb{C}^4$ . The converse holds when  $\varrho$  is X-shaped.

*Proof.* We consider  $W = X(s, t, u)$  with

$$s = \frac{1}{A(x, y)}x, \quad t = \frac{1}{A(x, y)}y, \quad u = -\frac{1}{C(z)}(z_1, z_2, z_3, \bar{z}_4).$$

By Proposition 3.4, we have

$$\begin{aligned}
B(u) &= \max_{\theta} \frac{|z_1 e^{i\theta} + z_4| + |z_2 e^{i\theta} + \bar{z}_3|}{C(z)} \\
&= 1 \\
&= \inf_{r>0} \frac{\sqrt{(x_1 r^{-1} + y_4 r)(x_4 r^{-1} + y_1 r)} + \sqrt{(x_2 r^{-1} + y_3 r)(x_3 r^{-1} + y_2 r)}}{A(x, y)} \\
&= A(s, t).
\end{aligned}$$

By Proposition 3.3, it follows that

$$0 \leq \langle \varrho, W \rangle = \frac{\sum_{i=1}^4 a_i x_i + \sum_{i=1}^4 b_i y_i}{A(x, y)} - \frac{2\mathcal{L}(\varrho, z)}{C(z)}.$$

For the converse, it suffices to show that  $\langle \varrho, W \rangle \geq 0$  for every X-shaped witness  $W$  by Proposition 3.1. We put  $W = X(x, y, -(z_1, z_2, z_3, \bar{z}_4))$ . We may assume without loss of generality that  $A(x, y) \geq 1 \geq B(z_1, z_2, z_3, \bar{z}_4)$  and  $\mathcal{L}(\varrho, z) \geq 0$ . Then we have

$$\begin{aligned} \langle \varrho, W \rangle &= \sum_{i=1}^4 a_i x_i + \sum_{i=1}^4 b_i y_i - 2\mathcal{L}(\varrho, z) \\ &\geq \frac{\sum_{i=1}^4 a_i x_i + \sum_{i=1}^4 b_i y_i}{A(x, y)} - \frac{2\mathcal{L}(\varrho, z)}{C(z)} \geq 0, \end{aligned}$$

as it was desired.  $\square$

Choosing special types of vectors  $x$  and  $y$  in Proposition 4.1 gives rise to the Gühne's necessary condition for separability. We include here our proof for completeness as well as motivation to prove sufficiency. We recall that the X-part of a separable state is again separable, and the following criteria involves only the X-part of a state.

**Theorem 4.2** (Gühne). *If  $\varrho$  is a three qubit separable state, then the inequality (3) holds for every  $z \in \mathbb{C}^4$ .*

*Proof.* It suffices to prove the required inequality, when  $c$  is a nonzero vector. By the PPT condition, all  $a_i, b_i$  are nonzero. Now, we fix  $i$  among 1, 2, 3, 4, and define  $x, y \in \mathbb{R}_+^4$  by

$$x_j = \begin{cases} \sqrt{b_i/a_i}, & j = i \\ 0, & j \neq i \end{cases}, \quad y_j = \begin{cases} \sqrt{a_i/b_i}, & j = i \\ 0, & j \neq i \end{cases}.$$

Then we have  $A(x, y) = 1$  and

$$\sum_{j=1}^4 a_j x_j + \sum_{j=1}^4 b_j y_j = 2\sqrt{a_i b_i},$$

which yields  $\mathcal{L}(\varrho, z) \leq C(z)\sqrt{a_i b_i}$ .

Next, we define  $x, y \in \mathbb{R}_+^4$  as follows:

$$x = \left( \sqrt[4]{a_1^{-3} b_2 b_3 a_4}, 0, 0, \sqrt[4]{a_1 b_2 b_3 a_4^{-3}} \right), \quad y = \left( 0, \sqrt[4]{a_1 b_2^{-3} b_3 a_4}, \sqrt[4]{a_1 b_2 b_3^{-3} a_4}, 0 \right).$$

Then we have

$$\begin{aligned} A(x, y) &= \inf_{r>0} \left( r^{-1} \sqrt[4]{a_1^{-1} b_2 b_3 a_4^{-1}} + r \sqrt[4]{a_1 b_2^{-1} b_3^{-1} a_4} \right) = 2, \\ \sum_{j=1}^4 a_j x_j + \sum_{j=1}^4 b_j y_j &= 4\sqrt[4]{a_1 b_2 b_3 a_4}, \end{aligned}$$

which yields  $\mathcal{L}(\varrho, z) \leq C(z)\sqrt[4]{a_1 b_2 b_3 a_4}$ . Finally, we use

$$x = \left( 0, \sqrt[4]{b_1 a_2^{-3} a_3 b_4}, \sqrt[4]{b_1 a_2 a_3^{-3} b_4}, 0 \right), \quad y = \left( \sqrt[4]{b_1^{-3} a_2 a_3 b_4}, 0, 0, \sqrt[4]{b_1 a_2 a_3 b_4^{-3}} \right)$$

in the exactly same way, to get the inequality  $\mathcal{L}(\varrho, z) \leq C(z)\sqrt[4]{b_1 a_2 a_3 b_4}$ .  $\square$



Now, we prove that the inequality (3) is equivalent to separability of GHZ diagonal states. The proof is similar to that of Proposition 4.1 if we use Theorem 3.2 instead of Proposition 3.1.

**Theorem 4.3.** *Let  $\varrho = X(a, a, c)$  be a three qubit GHZ diagonal state. Then,  $\varrho$  is separable if and only if the inequality (3) holds for every  $z \in \mathbb{R}^4$ .*

*Proof.* It remains to prove the ‘if’ part, and it suffices to show that  $\langle \varrho, W \rangle \geq 0$  for every GHZ diagonal witness  $W$  by Theorem 3.2. We put  $W = X(x, x, -z)$ . We may assume without loss of generality that  $A(x, x) \geq 1 \geq C(z)$  and  $\mathcal{L}(\varrho, z) \geq 0$ . We have

$$\begin{aligned} A(x, x) &= \inf_{r>0} \sqrt{(x_1 r^{-1} + x_4 r)(x_4 r^{-1} + x_1 r)} + \sqrt{(x_2 r^{-1} + x_3 r)(x_3 r^{-1} + x_2 r)} \\ &= \inf_{r>0} \sqrt{x_1 x_4 (r^{-2} + r^2) + x_1^2 + x_4^2} + \sqrt{x_2 x_3 (r^{-2} + r^2) + x_2^2 + x_3^2} \\ &= x_1 + x_2 + x_3 + x_4. \end{aligned}$$

Note that the minimums of two terms occur simultaneously when  $r = 1$ . Therefore, it follows that

$$\begin{aligned} \langle \varrho, W \rangle &= 2 \sum_{i=1}^4 a_i x_i - 2 \mathcal{L}(\varrho, z) \\ &\geq 2 \frac{\sum_{i=1}^4 a_i x_i}{A(x, x)} - 2 \frac{\mathcal{L}(\varrho, z)}{C(z)} \\ &= 2 \sum_{i=1}^4 a_i \frac{x_i}{x_1 + x_2 + x_3 + x_4} - 2 \frac{\mathcal{L}(\varrho, z)}{C(z)} \\ &\geq 2 \min\{a_1, a_2, a_3, a_4\} - 2 \frac{\mathcal{L}(\varrho, z)}{C(z)} \geq 0. \end{aligned}$$

This completes the proof.  $\square$

## 5. CHARACTERIZATION OF SEPARABILITY BY ENTRIES

In order to characterize separability of three qubit GHZ diagonal states in terms of entries, it suffices to find the maximum of the function

$$f(z_1, z_2, z_3, z_4) := \frac{c_1 z_1 + c_2 z_2 + c_3 z_3 + c_4 z_4}{C(z_1, z_2, z_3, z_4)} = \frac{c_1 z_1 + c_2 z_2 + c_3 z_3 + c_4 z_4}{\max_{\theta} (|z_1 e^{i\theta} + z_4| + |z_2 e^{i\theta} + z_3|)}$$

of real variables, by Theorem 4.3. We note that  $f$  is a continuous function defined on the domain  $\mathbb{R}^4 \setminus \{0\}$ , and enjoys the relations

$$(4) \quad f(\lambda z) = f(z) \text{ for each } \lambda > 0 \quad \text{and} \quad f(-z) = -f(z).$$

Hence,  $f$  has the maximum which occurs on the compact set  $\Delta = \{z : \sum_{i=1}^4 |z_i| = 1\}$ . In order to find this maximum, we first describe the function  $C$  in terms of real variables  $z_i$ 's.

Because the function  $C(z_1, z_2, z_3, z_4)$  is invariant under replacing two  $z_i$ 's by  $-z_i$ , it suffices to consider two cases  $z_1, z_2, z_3, z_4 \geq 0$  and  $z_1 < 0, z_2, z_3, z_4 > 0$ . In the former

case, it is trivial to see that  $C(z) = \sum_{i=1}^4 |z_i|$ . For the latter case, we put  $x = \cos \theta$  and define the function  $g : [-1, 1] \rightarrow \mathbb{R}$  by

$$g(x) = \sqrt{z_1^2 + z_4^2 - 2|z_1|z_4x} + \sqrt{z_2^2 + z_3^2 + 2z_2z_3x}, \quad x \in [-1, 1],$$

whose maximum is  $C(z)$ . By one variable calculus, one may check that

$$\begin{aligned} g'(x) \geq 0 &\iff z_2z_3\sqrt{z_1^2 + z_4^2 - 2|z_1|z_4x} \geq |z_1|z_4\sqrt{z_2^2 + z_3^2 + 2z_2z_3x} \\ &\iff x \leq \frac{z_2^2z_3^2(z_1^2 + z_4^2) - z_1^2z_4^2(z_2^2 + z_3^2)}{2|z_1|z_2z_3z_4(|z_1|z_4 + z_2z_3)} =: \alpha. \end{aligned}$$

If  $-1 < \alpha < 1$ , then  $g$  takes the maximum at  $\alpha$  with

$$\begin{aligned} C(z) = g(\alpha) &= \left( \sqrt{\frac{z_2z_3}{|z_1|z_4}} + \sqrt{\frac{|z_1|z_4}{z_2z_3}} \right) \sqrt{\frac{(|z_1|z_2 + z_3z_4)(|z_1|z_3 + z_2z_4)}{|z_1|z_4 + z_2z_3}} \\ &= \sqrt{\frac{(z_1z_2 - z_3z_4)(z_2z_4 - z_1z_3)(z_1z_4 - z_2z_3)}{-z_1z_2z_3z_4}}. \end{aligned}$$

We also have the following:

$$\alpha \leq -1 \iff \frac{1}{|z_1|} + \frac{1}{z_4} \leq \left| \frac{1}{z_2} - \frac{1}{z_3} \right|, \quad \alpha \geq 1 \iff \frac{1}{z_2} + \frac{1}{z_3} \leq \left| \frac{1}{|z_1|} - \frac{1}{z_4} \right|.$$

In the first case, we have  $C(z) = g(-1) = |z_1| + z_4 + |z_2 - z_3|$ . In the second case, we have  $C(z) = g(1) = ||z_1| - z_4| + z_2 + z_3$ .

We partition the domain of  $f$  by  $\mathbb{R}^4 \setminus \{0\} = \Omega^+ \sqcup \Omega^-$  with

$$\Omega^+ = \{z \in \mathbb{R}^4 \setminus \{0\} : z_1z_2z_3z_4 \geq 0\}, \quad \Omega^- = \{z \in \mathbb{R}^4 \setminus \{0\} : z_1z_2z_3z_4 < 0\}.$$

We also partition  $\Omega^-$  into the five regions  $\Omega_0^-, \Omega_1^-, \Omega_2^-, \Omega_3^-, \Omega_4^-$ :

$$\begin{aligned} \Omega_i^- &= \left\{ z \in \Omega^- : \frac{1}{|z_i|} \geq \sum_{j \neq i} \frac{1}{|z_j|} \right\}, \quad i = 1, 2, 3, 4, \\ \Omega_0^- &= \Omega^- \setminus (\sqcup_{i=1}^4 \Omega_i^-) = \left\{ z \in \Omega^- : \frac{1}{|z_i|} < \sum_{j \neq i} \frac{1}{|z_j|}, \quad i = 1, 2, 3, 4 \right\}. \end{aligned}$$

Note that  $z \in \Omega^-$  belongs to  $\Omega_0^-$  if and only if the numbers  $\frac{1}{|z_i|}$  with  $i = 1, 2, 3, 4$  make a quadrangle. In the case of  $z_1 < 0$  and  $z_2, z_3, z_4 > 0$ , we have  $\alpha \geq 1$  for  $z \in \Omega_1^-$  or  $z \in \Omega_4^-$ , while  $\alpha \leq -1$  for  $z \in \Omega_2^-$  or  $z \in \Omega_3^-$ . In each case,  $C(z)$  is equal to

$$-|z_1| + z_2 + z_3 + z_4, \quad |z_1| + z_2 + z_3 - z_4, \quad |z_1| - z_2 + z_3 + z_4, \quad |z_1| + z_2 - z_3 + z_4,$$

respectively. We also have

$$\begin{aligned} (5) \quad -1 < \alpha < 1 &\iff \frac{1}{|z_1|} + \frac{1}{|z_4|} > \left| \frac{1}{|z_2|} - \frac{1}{|z_3|} \right|, \quad \frac{1}{|z_2|} + \frac{1}{|z_3|} > \left| \frac{1}{|z_1|} - \frac{1}{|z_4|} \right| \\ &\iff z \in \Omega_0^-. \end{aligned}$$

We summarize as follows:

**Proposition 5.1.** *For  $z \in \mathbb{R}^4 \setminus \{0\}$ , we have*

$$C(z) = \begin{cases} |z_1| + |z_2| + |z_3| + |z_4|, & z \in \Omega^+, \\ |z_1| + |z_2| + |z_3| + |z_4| - 2|z_i|, & z \in \Omega_i^- \ (i = 1, 2, 3, 4), \\ \sqrt{\frac{(z_1 z_2 - z_3 z_4)(z_2 z_4 - z_1 z_3)(z_1 z_4 - z_2 z_3)}{-z_1 z_2 z_3 z_4}}, & z \in \Omega_0^-. \end{cases}$$

We also partition  $\Omega^-$  into the eight domains  $\Omega^\sigma$ , where  $\sigma$  is one of:

$$- + + +, + - + +, + + - +, + + + -, + - - -, - + - -, - - + -, - - - +,$$

according to the signs of  $z_1, z_2, z_3$  and  $z_4$ . We put

$$\Omega_i^\sigma := \Omega_i^- \cap \Omega^\sigma, \quad i = 0, 1, 2, 3, 4.$$

In order to understand the global behavior of the function  $f$ , we consider the boundary

$$B_i^\sigma := \left\{ z \in \Omega^\sigma : \frac{1}{|z_i|} = \sum_{j \neq i} \frac{1}{|z_j|} \right\}$$

between  $\Omega_0^\sigma$  and  $\Omega_i^\sigma$  for  $i = 1, 2, 3, 4$ . For example,  $B_1^{-+++}$  consists of  $z \in \mathbb{R}^4$  satisfying

$$z_1 < 0, \ z_2, z_3, z_4 > 0, \quad z_1 = -\frac{z_2 z_3 z_4}{z_2 z_3 + z_3 z_4 + z_4 z_2}.$$

If we fix two of  $z_2, z_3, z_4$  and take another  $z_i \rightarrow 0^+$ , then we have  $z_1 \rightarrow 0^-$ . This means that every point on the plane  $z_1 = z_2 = 0$ ,  $z_1 = z_3 = 0$  or  $z_1 = z_4 = 0$  with  $z_i \geq 0$  ( $i = 2, 3, 4$ ) is a limit point of  $B_1^{-+++}$ .

By the relation (4), we may restrict the domain of  $f$  on the set  $\Delta$ . Then the intersection  $\Omega^\sigma \cap \Delta$  with  $\Omega^\sigma$  is a tetrahedron, and  $B_i^\sigma \cap \Delta$  is a two-dimensional surface in the tetrahedron. For example, the set  $\Omega^{-+++} \cap \Delta$  is the tetrahedron with four extreme points  $-E_1, E_2, E_3$  and  $E_4$ , and the surface  $B_1^{-+++} \cap \Delta$  consists of  $z \in \mathbb{R}^4$  satisfying

$$z_1 < 0, \ z_2, z_3, z_4 > 0, \quad \frac{1}{z_1} + \frac{1}{z_2} + \frac{1}{z_3} + \frac{1}{z_4} = 0, \quad -z_1 + z_2 + z_3 + z_4 = 1.$$

Limit points of the surface include the three edges of the face  $F_1$  with extreme points  $E_2, E_3, E_4$ . This surface is near from the face  $F_1$ , and far from the extreme point  $-E_1$ . The maximum distance from the surface  $B_1^{-+++} \cap \Delta$  to the face  $F_1$  is given by

$$\|(-\frac{1}{10}, \frac{3}{10}, \frac{3}{10}, \frac{3}{10}) - (0, \frac{1}{3}, \frac{1}{3}, \frac{1}{3})\| = \frac{1}{5\sqrt{3}}.$$

The each piece of the region  $\Omega_0^\sigma$  in  $\Delta$  occupies the central part of the corresponding tetrahedron, and touches all the edges and extreme points of the tetrahedron, but is apart from the four faces with dimension two.

Since  $f$  is a fraction of linear functions on each  $\Omega_i^\sigma$  with  $i = 1, 2, 3, 4$ , all its partial derivatives never vanish on them, and so  $f$  has no extreme value on the interior of  $\sqcup_{i=1}^4 \Omega_i^-$ . Therefore, we see that the maximum value of  $f$  occurs on  $\Omega^+$ ,  $B_i^\sigma$  or  $\Omega_0^-$ . If the maximum occurs on  $\Omega^+$  then we have  $\max f(z) = \max_i |c_i|$ , in which case the separability of  $\varrho$  is equivalent to the condition of PPT by Theorem 4.3.

Now, we consider the function  $f(z)$  with the third expression of  $C(z)$ , and suppose that  $s = (s_1, s_2, s_3, s_4) \in \Omega_0^-$  is a critical point of  $f$ . With the notation  $t_i = 1/s_i$ , we have

$$(6) \quad \begin{aligned} t_1 &= c_1(-c_1^2 + c_2^2 + c_3^2 + c_4^2) - 2c_2c_3c_4, \\ t_2 &= c_2(+c_1^2 - c_2^2 + c_3^2 + c_4^2) - 2c_1c_3c_4, \\ t_3 &= c_3(+c_1^2 + c_2^2 - c_3^2 + c_4^2) - 2c_1c_2c_4, \\ t_4 &= c_4(+c_1^2 + c_2^2 + c_3^2 - c_4^2) - 2c_1c_2c_3, \end{aligned}$$

up to nonzero scalar multiplications. See Appendix for the details. One may also check

$$\begin{aligned} f(s)^2 &= \frac{4(c_1c_2 - c_3c_4)(c_1c_3 - c_2c_4)(c_1c_4 - c_2c_3)}{(c_1 + c_2 + c_3 + c_4)(c_1 + c_2 - c_3 - c_4)(c_1 - c_2 - c_3 + c_4)(c_1 - c_2 + c_3 - c_4)} \\ &= \frac{(\lambda_5\lambda_6 + \lambda_7\lambda_8)(\lambda_5\lambda_7 + \lambda_6\lambda_8)(\lambda_5\lambda_8 + \lambda_6\lambda_7)}{8^2\lambda_5\lambda_6\lambda_7\lambda_8} \end{aligned}$$

which appears in the sufficient condition of G uhne (2). We are going to look for the condition with which the critical point  $s = (s_1, s_2, s_3, s_4)$  belongs to  $\Omega_0^-$ . To do this, we note by calculation the following relations between  $t_i$  and  $\lambda_j$ :

$$\begin{aligned} (t_2 + t_3)^2 - (t_1 + t_4)^2 &= \frac{1}{2^6}\lambda_5\lambda_8(\lambda_6\lambda_7)^2, \\ (t_1 - t_4)^2 - (t_2 - t_3)^2 &= \frac{1}{2^6}\lambda_6\lambda_7(\lambda_5\lambda_8)^2. \end{aligned}$$

Since  $s = (s_1, s_2, s_3, s_4) \in \Omega^-$ , we have  $(t_1t_4)(t_2t_3) < 0$ . We first consider the case  $t_1t_4 > 0$  and  $t_2t_3 < 0$ . In this case, we have

$$\begin{aligned} |t_2| + |t_3| > ||t_1| - |t_4|| &\iff (t_2 - t_3)^2 > (t_1 - t_4)^2 \iff \lambda_6\lambda_7 < 0, \\ |t_1| + |t_4| > ||t_2| - |t_3|| &\iff (t_1 + t_4)^2 > (t_2 + t_3)^2 \iff \lambda_5\lambda_8 < 0. \end{aligned}$$

In case of  $t_1t_4 < 0$  and  $t_2t_3 > 0$ , we also have

$$\begin{aligned} |t_2| + |t_3| > ||t_1| - |t_4|| &\iff (t_2 + t_3)^2 > (t_1 + t_4)^2 \iff \lambda_5\lambda_8 > 0, \\ |t_1| + |t_4| > ||t_2| - |t_3|| &\iff (t_1 - t_4)^2 > (t_2 - t_3)^2 \iff \lambda_6\lambda_7 > 0. \end{aligned}$$

By (5), we see that  $s \in \Omega_0^-$  if and only if

$$t_1t_4 > 0, t_2t_3 < 0, \lambda_6\lambda_7 < 0, \lambda_5\lambda_8 < 0 \text{ or } t_1t_4 < 0, t_2t_3 > 0, \lambda_6\lambda_7 > 0, \lambda_5\lambda_8 > 0$$

if and only if  $\lambda_5\lambda_6\lambda_7\lambda_8 > 0$  and

$$(7) \quad t_1t_4\lambda_6\lambda_7 < 0 \quad \text{and} \quad t_2t_3\lambda_5\lambda_8 > 0.$$

Summing up, we have seen that the function  $f$  with the third expression of  $C(z)$  has a critical value on  $\Omega_0^-$  if and only if the inequality  $\lambda_5\lambda_6\lambda_7\lambda_8 > 0$  together with the condition (7) holds. Now, we are ready to state and prove the following, which correct a result in [22].

**Theorem 5.2.** *Let  $\varrho = X(a, a, c)$  be a GHZ diagonal state. Suppose that  $\lambda_5, \lambda_6, \lambda_7, \lambda_8$  and  $t_1, t_2, t_3, t_4$  are given by (1) and (6), respectively. Then we have the following:*

- (i) *if  $\lambda_5\lambda_6\lambda_7\lambda_8 \leq 0$ , then  $\varrho$  is separable if and only if it is of PPT;*

- (ii) if  $\lambda_5\lambda_6\lambda_7\lambda_8 > 0$  and (7) does not hold, then  $\varrho$  is separable if and only if it is of PPT;
- (iii) if  $\lambda_5\lambda_6\lambda_7\lambda_8 > 0$  and (7) holds, then  $\varrho$  is separable if and only if the inequality (2) holds.

*Proof.* We first consider the behavior of the function  $f$  on the surface  $B_i^\sigma \cap \Delta$ , say  $B_1^{-+++} \cap \Delta$ . To do this, we denote by  $f_2$  and  $f_3$  the function  $f$  with the second and third expression of  $C(z)$  in Proposition 5.1. We take the line segment

$$z(t) = (1-t)(-E_1) + t(0, \omega_2, \omega_3, \omega_4) = (t-1, t\omega_2, t\omega_3, t\omega_4), \quad 0 \leq t \leq 1$$

between the extreme point  $-E_1$  and a point  $(0, \omega_2, \omega_3, \omega_4)$  on the opposite face  $F_1$ , with  $\omega_2 + \omega_3 + \omega_4 = 1$  and  $\omega_i \geq 0$ . The line segment meets the surface  $B_1^{-+++} \cap \Delta$  at

$$t_0 = \frac{\omega_2\omega_3 + \omega_3\omega_4 + \omega_4\omega_2}{\omega_2\omega_3\omega_4 + \omega_2\omega_3 + \omega_3\omega_4 + \omega_4\omega_2}.$$

One may check that the derivatives of  $f_2(z(t))$  and  $f_3(z(t))$  at  $t = t_0$  are positive scalar multiples of  $c_1 - c_2\omega_2 - c_3\omega_3 - c_4\omega_4$ . Therefore, we see that the function  $f$  has no extreme value on the surface  $B_1^{-+++} \cap \Delta$  possibly except on the curve

$$\{(t_0 - 1, t_0\omega_2, t_0\omega_3, t_0\omega_4) : c_2\omega_2 + c_3\omega_3 + c_4\omega_4 = c_1, \omega_2 + \omega_3 + \omega_4 = 1, \omega_i \geq 0\},$$

where  $f$  has the constant value  $c_1$ . The other cases can be handled in the same way to see that possible extreme values are  $\pm c_i$ .

Suppose that the assumption of (i) or (ii) holds. Then we see by the above argument that the global maximum of  $f$  is  $\max |c_i|$ . Therefore, we have the required results by Theorem 4.3. In case of (iii), we know that the maximum of  $f$  is  $\max |c_i|$  or the number in the inequality (2). One may check that the square of this number is equal to  $c_i^2 + \frac{2^4 t_i^2}{\lambda_5 \lambda_6 \lambda_7 \lambda_8}$  for each  $i = 1, 2, 3, 4$ . Therefore, we conclude that the maximum of  $f$  is the number in (2), when  $\lambda_5 \lambda_6 \lambda_7 \lambda_8 > 0$ . This completes the proof by Theorem 4.3 again.  $\square$

The case (i) is just Kay's criterion. The case (iii) tells us that Gühne's sufficient condition is also necessary under the condition (7). The case (ii) is most interesting. This case shows that separability of  $\varrho$  may be equivalent to PPT even though the Kay's condition  $\lambda_5 \lambda_6 \lambda_7 \lambda_8 < 0$  is not satisfied. This case also provides examples of separable states violating Gühne's sufficient condition.

Motivated by Kay's example in [18], we consider the family of GHZ diagonal states

$$\varrho_{p,q} = \frac{1}{8} X(\mathbf{1}, \mathbf{1}, (p, p, q, p))$$

where  $\mathbf{1} = (1, 1, 1, 1)$ . This is really a state if and only if  $\max\{|p|, |q|\} \leq 1$  if and only if it is of PPT. In this case, we have

$$\begin{aligned} t_1 = t_2 = t_4 &= \frac{1}{8^3} p(p-q)^2, & t_3 &= -\frac{1}{8^3} (2p+q)(p-q)^2, \\ \lambda_5 &= \frac{1}{4} (3p+q), & \lambda_6 = \lambda_8 &= \frac{1}{4} (-p+q), & \lambda_7 &= \frac{1}{4} (p-q). \end{aligned}$$

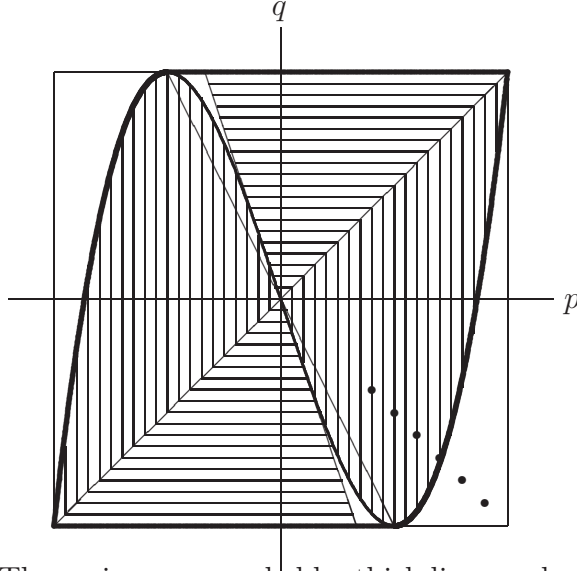


FIGURE 1. The region surrounded by thick lines and curves denotes separable states among  $\varrho_{p,q}$ . States outside of this curves in the box are PPT entanglement. Especially, dots denote Kay's examples of one parameter family to find PPT entanglement among GHZ diagonal states. Kay's criterion works on the parts with horizontal lines. The parts with vertical lines represent separable states satisfying Gühne's sufficient condition. States in remaining parts violate this condition even though they are separable and satisfy  $\lambda_5\lambda_6\lambda_7\lambda_8 > 0$ .

Therefore, we have the following:

- the case (i) occurs if and only if  $(p - q)(3p + q) \leq 0$ ,
- the case (ii) occurs if and only if  $(p - q)(3p + q) > 0$  and  $p(2p + q) \leq 0$ ,
- the case (iii) occurs if and only if  $(p - q)(3p + q) > 0$  and  $p(2p + q) > 0$ ,
- the inequality (2) holds if and only if  $(p - q)(3p + q) > 0$  and  $\frac{4p^3}{3p+q} \leq 1$ .

See Figure 1.

In multi-partite systems, we note that there are various notions of separability and entanglement according to partitions of systems. For example, we say that a multi-partite state is fully bi-separable if it is separable as a bi-partite state with respect to every bi-partition of systems. Characterization of full bi-separability and corresponding witnesses are given for general multi-qubit X-shaped states [23]. We note that only absolute values of anti-diagonal entries involved in these criteria. On the other hand, the arguments of anti-diagonal entries play a key role in the characterization of witnesses corresponding (full) separability, as we have seen in Proposition 3.3. In this regard, it would be very interesting to get a characterization for separability of general X-shaped three qubit states when the anti-diagonals have complex entries.

## 6. APPENDIX

Suppose that  $s = (s_1, s_2, s_3, s_4)$  is a critical point of the function

$$f(z_1, z_2, z_3, z_4) = \frac{c_1 z_1 + c_2 z_2 + c_3 z_3 + c_4 z_4}{\sqrt{\frac{(z_1 z_2 - z_3 z_4)(z_2 z_4 - z_1 z_3)(z_1 z_4 - z_2 z_3)}{-z_1 z_2 z_3 z_4}}}$$

when  $z \in \Omega_0^-$ . From

$$\log C(z) = \frac{1}{2}(\log |z_1 z_2 - z_3 z_4| + \log |z_2 z_4 - z_1 z_3| + \log |z_1 z_4 - z_2 z_3| - \log(-z_1 z_2 z_3 z_4)),$$

we get logarithmic derivatives

$$\begin{aligned} 2 \frac{\frac{\partial C}{\partial z_1}(z)}{C(z)} &= + \frac{z_2}{z_1 z_2 - z_3 z_4} - \frac{z_3}{z_2 z_4 - z_1 z_3} + \frac{z_4}{z_1 z_4 - z_2 z_3} - \frac{1}{z_1}, \\ 2 \frac{\frac{\partial C}{\partial z_2}(z)}{C(z)} &= + \frac{z_1}{z_1 z_2 - z_3 z_4} + \frac{z_4}{z_2 z_4 - z_1 z_3} - \frac{z_3}{z_1 z_4 - z_2 z_3} - \frac{1}{z_2}, \\ 2 \frac{\frac{\partial C}{\partial z_3}(z)}{C(z)} &= - \frac{z_4}{z_1 z_2 - z_3 z_4} - \frac{z_1}{z_2 z_4 - z_1 z_3} - \frac{z_2}{z_1 z_4 - z_2 z_3} - \frac{1}{z_3}, \\ 2 \frac{\frac{\partial C}{\partial z_4}(z)}{C(z)} &= - \frac{z_3}{z_1 z_2 - z_3 z_4} + \frac{z_2}{z_2 z_4 - z_1 z_3} + \frac{z_1}{z_1 z_4 - z_2 z_3} - \frac{1}{z_4}. \end{aligned}$$

We also consider the logarithmic derivatives of  $f$  at  $s$  as

$$0 = \frac{\frac{\partial f}{\partial z_i}(s)}{f(s)} = \frac{c_i}{c_1 s_1 + c_2 s_2 + c_3 s_3 + c_4 s_4} - \frac{\frac{\partial C}{\partial z_i}(s)}{C(s)}.$$

Combining the above, we obtain simultaneous equations

$$(8) \quad \frac{2c_1 s_1}{c_1 s_1 + c_2 s_2 + c_3 s_3 + c_4 s_4} = + \frac{s_1 s_2}{s_1 s_2 - s_3 s_4} - \frac{s_1 s_3}{s_2 s_4 - s_1 s_3} + \frac{s_1 s_4}{s_1 s_4 - s_2 s_3} - 1,$$

$$(9) \quad \frac{2c_2 s_2}{c_1 s_1 + c_2 s_2 + c_3 s_3 + c_4 s_4} = + \frac{s_1 s_2}{s_1 s_2 - s_3 s_4} + \frac{s_2 s_4}{s_2 s_4 - s_1 s_3} - \frac{s_2 s_3}{s_1 s_4 - s_2 s_3} - 1,$$

$$(10) \quad \frac{2c_3 s_3}{c_1 s_1 + c_2 s_2 + c_3 s_3 + c_4 s_4} = - \frac{s_3 s_4}{s_1 s_2 - s_3 s_4} - \frac{s_1 s_3}{s_2 s_4 - s_1 s_3} - \frac{s_2 s_3}{s_1 s_4 - s_2 s_3} - 1,$$

$$(11) \quad \frac{2c_4 s_4}{c_1 s_1 + c_2 s_2 + c_3 s_3 + c_4 s_4} = - \frac{s_3 s_4}{s_1 s_2 - s_3 s_4} + \frac{s_2 s_4}{s_2 s_4 - s_1 s_3} + \frac{s_1 s_4}{s_1 s_4 - s_2 s_3} - 1.$$

Taking  $\frac{(8)+(9)}{(10)+(11)}$ ,  $\frac{(8)+(10)}{(9)+(11)}$ ,  $\frac{(8)+(11)}{(9)+(10)}$ , we have

$$\frac{c_1 s_1 + c_2 s_2}{c_3 s_3 + c_4 s_4} = - \frac{s_1 s_2}{s_3 s_4}, \quad \frac{c_1 s_1 + c_3 s_3}{c_2 s_2 + c_4 s_4} = - \frac{s_1 s_3}{s_2 s_4}, \quad \frac{c_1 s_1 + c_4 s_4}{c_2 s_2 + c_3 s_3} = - \frac{s_1 s_4}{s_2 s_3},$$

equivalently the system of linear equations

$$c_2 \omega_1 + c_1 \omega_2 + c_4 \omega_3 + c_3 \omega_4 = 0,$$

$$c_3 \omega_1 + c_4 \omega_2 + c_1 \omega_3 + c_2 \omega_4 = 0,$$

$$c_4 \omega_1 + c_3 \omega_2 + c_2 \omega_3 + c_1 \omega_4 = 0$$

if we put

$$\omega_1 := s_2 s_3 s_4, \quad \omega_2 := s_1 s_3 s_4, \quad \omega_3 := s_1 s_2 s_4, \quad \omega_4 := s_1 s_2 s_3.$$

We take

$$\omega_4 = - \begin{vmatrix} c_2 & c_1 & c_4 \\ c_3 & c_4 & c_1 \\ c_4 & c_3 & c_2 \end{vmatrix} = c_4(-c_1^2 - c_2^2 - c_3^2 + c_4^2) + 2c_1c_2c_3.$$

considering the relation (4). Then, we have

$$\begin{aligned} \omega_1 &= \begin{vmatrix} c_3 & c_1 & c_4 \\ c_2 & c_4 & c_1 \\ c_1 & c_3 & c_2 \end{vmatrix} = c_1(+c_1^2 - c_2^2 - c_3^2 - c_4^2) + 2c_2c_3c_4, \\ \omega_2 &= \begin{vmatrix} c_2 & c_3 & c_4 \\ c_3 & c_2 & c_1 \\ c_4 & c_1 & c_2 \end{vmatrix} = c_2(-c_1^2 + c_2^2 - c_3^2 - c_4^2) + 2c_1c_3c_4, \\ \omega_3 &= \begin{vmatrix} c_2 & c_1 & c_3 \\ c_3 & c_4 & c_2 \\ c_4 & c_3 & c_1 \end{vmatrix} = c_3(-c_1^2 - c_2^2 + c_3^2 - c_4^2) + 2c_1c_2c_4. \end{aligned}$$

Hence, (6) follows from the relation

$$-\frac{1}{s_1s_2s_3s_4}s_i = -\frac{1}{\omega_i}.$$

Here, we may ignore the common positive scalar multiple  $-1/s_1s_2s_3s_4$  by (4).

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